Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 08:49 PM JST

PDB ID	:	7DFB
Title	:	Crystal of Arrestin2-V2Rpp-6-7-Fab30 complex
Authors	:	Sun, J.P.; Yu, X.; Xiao, P.; He, Q.T.; Lin, J.Y.; Zhu, Z.L.
Deposited on	:	2020-11-06
Resolution	:	3.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

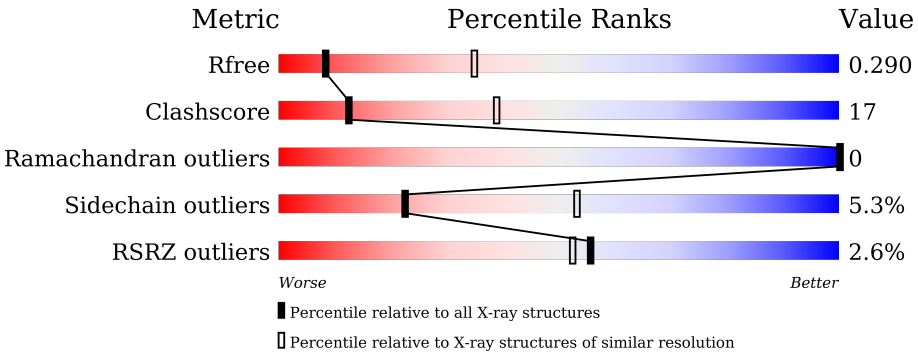
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	426	% 52% 30% • 16%
2	V	23	43% 35% 9% 13%
3	L	227	4% 58% 33% • 7%
4	H	249	3% 59% 26% • 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5913 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-arrestin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2702	1728	462	502	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P17870
A	420	GLU	-	expression tag	UNP P17870
A	421	HIS	-	expression tag	UNP P17870
A	422	HIS	-	expression tag	UNP P17870
A	423	HIS	-	expression tag	UNP P17870
A	424	HIS	-	expression tag	UNP P17870
A	425	HIS	-	expression tag	UNP P17870
A	426	HIS	-	expression tag	UNP P17870

- Molecule 2 is a protein called V2Rpp-6-7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	V	20	Total	C	N	O	P	S	0	0	0
			151	75	21	48	6	1			

- Molecule 3 is a protein called FAB30 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1550	970	254	321	5			

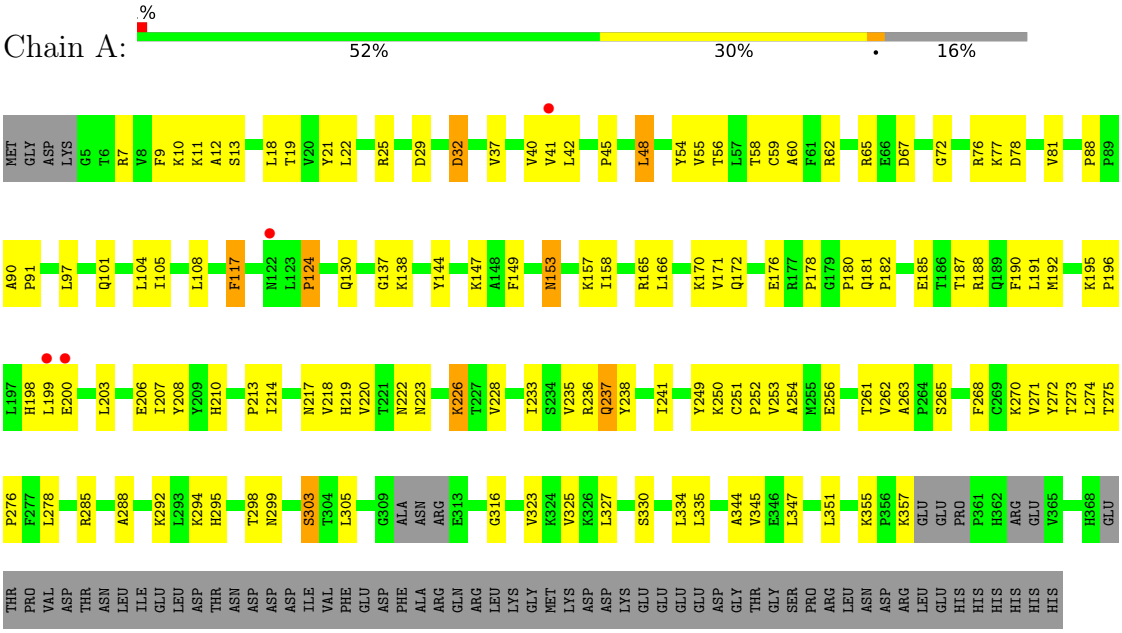
- Molecule 4 is a protein called FAB30 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	213	Total	C	N	O	S	0	0	0
			1510	957	253	295	5			

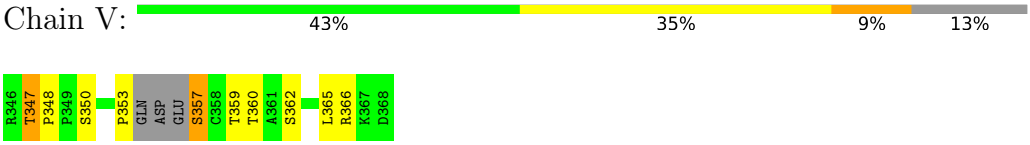
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

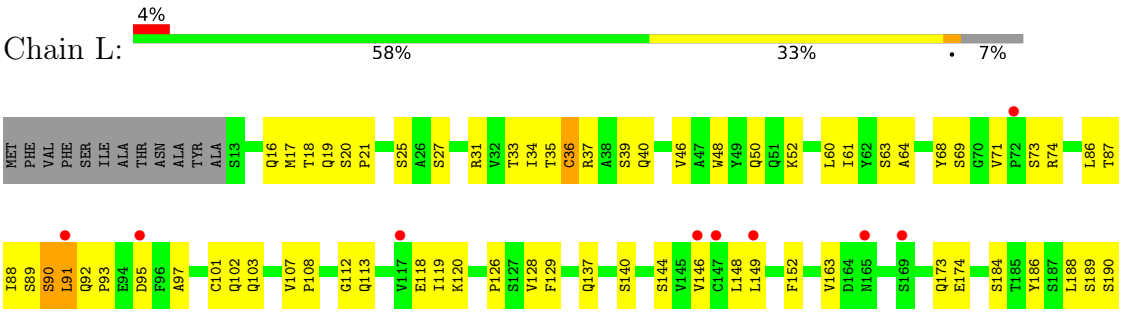
• Molecule 1: Beta-arrestin-1

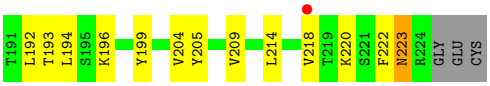


• Molecule 2: V2Rpp-6-7



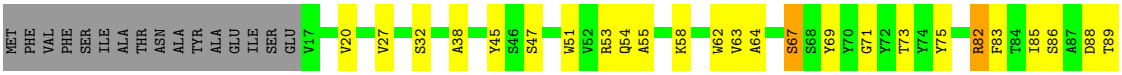
• Molecule 3: FAB30 LIGHT CHAIN

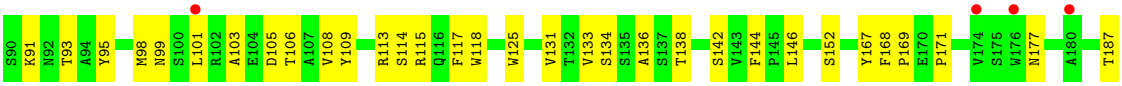


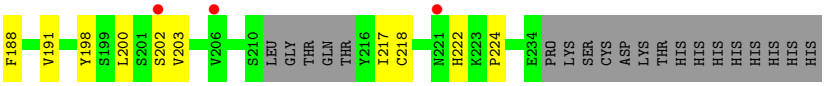


• Molecule 4: FAB30 HEAVY CHAIN

Chain H:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.48Å 116.88Å 143.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.36 – 3.28 45.36 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.36-3.28) 99.1 (45.36-3.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.231 , 0.290 0.232 , 0.290	Depositor DCC
R_{free} test set	750 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	110.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 71.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5913	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.52	1/2757 (0.0%)	0.69	0/3751
2	V	0.44	0/85	0.70	0/107
3	L	0.46	0/1581	0.66	0/2158
4	H	0.49	0/1550	0.71	0/2124
All	All	0.49	1/5973 (0.0%)	0.69	0/8140

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	GLU	C-N	-5.22	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2702	0	2697	93	0
2	V	151	0	104	5	0
3	L	1550	0	1463	57	0
4	H	1510	0	1353	50	0
All	All	5913	0	5617	194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:82:ARG:HG2	4:H:82:ARG:HH11	1.40	0.85
4:H:134:SER:HB3	4:H:168:PHE:HZ	1.42	0.84
1:A:62:ARG:HG2	1:A:76:ARG:HG2	1.69	0.74
1:A:40:VAL:HG22	1:A:104:LEU:HD13	1.70	0.73
3:L:18:THR:HG22	3:L:113:GLN:HE22	1.54	0.73
1:A:42:LEU:HD22	1:A:108:LEU:HD13	1.71	0.72
3:L:90:SER:O	3:L:92:GLN:NE2	2.22	0.72
1:A:292:LYS:HG2	1:A:298:THR:OG1	1.88	0.72
3:L:146:VAL:HG11	4:H:146:LEU:HD13	1.73	0.71
4:H:134:SER:HB3	4:H:168:PHE:CZ	2.26	0.69
4:H:53:ARG:HB2	4:H:109:TYR:CE1	2.29	0.67
1:A:233:ILE:HD13	1:A:325:VAL:HG22	1.76	0.66
3:L:68:TYR:HB3	3:L:71:VAL:HG21	1.78	0.66
3:L:214:LEU:HD22	3:L:218:VAL:HG21	1.78	0.66
3:L:48:TRP:HB2	3:L:61:ILE:HG22	1.77	0.66
3:L:128:VAL:HG21	3:L:209:VAL:HG21	1.76	0.65
4:H:82:ARG:HH11	4:H:82:ARG:CG	2.10	0.65
1:A:213:PRO:HA	1:A:275:THR:HG22	1.78	0.65
1:A:12:ALA:HA	1:A:19:THR:HA	1.77	0.65
3:L:34:ILE:HD12	3:L:86:LEU:HD23	1.78	0.64
1:A:171:VAL:HG22	1:A:172:GLN:H	1.62	0.63
1:A:29:ASP:HB2	1:A:170:LYS:HE2	1.80	0.63
1:A:355:LYS:HD2	1:A:357:LYS:HE3	1.80	0.63
3:L:204:VAL:HG13	3:L:204:VAL:O	1.98	0.62
1:A:203:LEU:HD21	1:A:323:VAL:HG11	1.81	0.62
4:H:55:ALA:HB3	4:H:58:LYS:HB2	1.80	0.62
3:L:199:TYR:HH	3:L:222:PHE:HE2	1.47	0.61
1:A:222:ASN:O	1:A:265:SER:HA	2.00	0.61
3:L:31:ARG:HG2	3:L:89:SER:HA	1.82	0.60
4:H:103:ALA:O	4:H:106:THR:HG22	2.02	0.59
1:A:182:PRO:HG2	1:A:203:LEU:HB2	1.84	0.59
1:A:217:ASN:HA	1:A:271:VAL:HG12	1.84	0.59
1:A:185:GLU:HB2	1:A:198:HIS:HE1	1.68	0.58
3:L:33:THR:HG22	3:L:87:THR:HA	1.86	0.58
3:L:107:VAL:N	3:L:108:PRO:HD2	2.19	0.58
1:A:235:VAL:HG11	1:A:276:PRO:HG3	1.85	0.57
4:H:142:SER:HB3	4:H:144:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PRO:HG2	1:A:91:PRO:HD3	1.86	0.57
3:L:92:GLN:HB3	3:L:93:PRO:HD2	1.85	0.57
1:A:199:LEU:HD13	1:A:327:LEU:HD11	1.87	0.56
4:H:75:TYR:OH	4:H:85:ILE:N	2.33	0.56
3:L:18:THR:O	3:L:36:CYS:HA	2.06	0.55
4:H:53:ARG:NH1	4:H:105:ASP:HA	2.22	0.55
3:L:204:VAL:HB	3:L:223:ASN:HD21	1.71	0.55
4:H:118:TRP:CD1	4:H:118:TRP:N	2.71	0.55
1:A:13:SER:OG	1:A:18:LEU:HB2	2.07	0.55
4:H:67:SER:O	4:H:71:GLY:N	2.39	0.55
1:A:54:TYR:HB2	1:A:149:PHE:CZ	2.43	0.55
3:L:27:SER:HB3	3:L:120:LYS:HE2	1.89	0.54
3:L:16:GLN:H	3:L:39:SER:HB2	1.73	0.54
1:A:299:ASN:HB3	4:H:117:PHE:HE1	1.72	0.54
1:A:200:GLU:HB2	1:A:219:HIS:HB3	1.89	0.54
3:L:118:GLU:HG3	3:L:186:TYR:OH	2.08	0.54
3:L:46:VAL:HG13	3:L:102:GLN:O	2.08	0.54
3:L:50:GLN:HB3	3:L:60:LEU:HD11	1.89	0.54
1:A:77:LYS:NZ	2:V:347:TPO:HG23	2.23	0.53
1:A:210:HIS:HB3	4:H:117:PHE:CZ	2.44	0.53
1:A:18:LEU:HD22	1:A:41:VAL:CG2	2.38	0.53
3:L:19:GLN:HA	3:L:35:THR:O	2.09	0.53
1:A:124:PRO:HG3	1:A:316:GLY:HA3	1.89	0.53
4:H:188:PHE:O	4:H:200:LEU:HD11	2.09	0.53
1:A:78:ASP:OD1	1:A:78:ASP:N	2.42	0.52
3:L:119:ILE:HD12	3:L:184:SER:OG	2.10	0.52
1:A:237:GLN:N	1:A:251:CYS:O	2.42	0.52
3:L:126:PRO:HB3	3:L:152:PHE:CD2	2.43	0.52
1:A:222:ASN:ND2	1:A:263:ALA:O	2.43	0.52
3:L:20:SER:HB2	3:L:35:THR:HG23	1.91	0.52
4:H:82:ARG:HG2	4:H:82:ARG:NH1	2.19	0.52
3:L:149:LEU:HB2	3:L:188:LEU:HB3	1.92	0.52
4:H:138:THR:HG23	4:H:169:PRO:HG3	1.92	0.51
1:A:157:LYS:O	1:A:158:ILE:HD13	2.11	0.51
4:H:88:ASP:HB2	4:H:95:TYR:HE2	1.76	0.51
1:A:153:ASN:N	1:A:153:ASN:OD1	2.43	0.51
1:A:295:HIS:NE2	2:V:353:PRO:HG3	2.25	0.51
1:A:149:PHE:CD2	1:A:158:ILE:HD12	2.46	0.50
3:L:222:PHE:CD2	3:L:222:PHE:C	2.85	0.50
1:A:45:PRO:HA	1:A:48:LEU:HB3	1.94	0.50
1:A:237:GLN:OE1	1:A:288:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:204:VAL:CB	3:L:223:ASN:HD21	2.25	0.50
1:A:187:THR:HG23	1:A:198:HIS:HA	1.93	0.50
1:A:238:TYR:CE1	1:A:250:LYS:HB3	2.47	0.50
1:A:188:ARG:HD2	1:A:190:PHE:CE1	2.46	0.50
1:A:196:PRO:O	1:A:223:ASN:HB2	2.11	0.50
4:H:83:PHE:CE1	4:H:98:MET:HB3	2.47	0.50
1:A:72:GLY:HA2	1:A:137:GLY:HA3	1.94	0.49
1:A:181:GLN:HG3	1:A:203:LEU:O	2.11	0.49
1:A:206:GLU:O	1:A:206:GLU:HG2	2.12	0.49
3:L:148:LEU:HD11	4:H:203:VAL:HG21	1.93	0.49
1:A:236:ARG:HA	1:A:252:PRO:HA	1.94	0.49
4:H:136:ALA:HB3	4:H:168:PHE:CE2	2.47	0.49
4:H:187:THR:HG23	4:H:202:SER:HB2	1.95	0.48
1:A:60:ALA:HA	1:A:78:ASP:HA	1.95	0.48
1:A:65:ARG:HG2	1:A:67:ASP:OD1	2.13	0.47
1:A:236:ARG:NH1	1:A:250:LYS:HE3	2.28	0.47
3:L:174:GLU:HA	3:L:190:SER:HA	1.96	0.47
1:A:97:LEU:HB2	1:A:101:GLN:HB2	1.95	0.47
3:L:17:MET:HA	3:L:37:ARG:O	2.14	0.47
1:A:191:LEU:HD23	1:A:334:LEU:CD2	2.44	0.47
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.74	0.47
4:H:177:ASN:N	4:H:217:ILE:O	2.40	0.47
1:A:37:VAL:HG13	1:A:117:PHE:HB2	1.97	0.46
3:L:74:ARG:HD2	3:L:88:ILE:HD11	1.96	0.46
4:H:222:HIS:CD2	4:H:224:PRO:HD2	2.50	0.46
1:A:233:ILE:CD1	1:A:325:VAL:HG22	2.42	0.46
3:L:48:TRP:CZ3	3:L:101:CYS:HB3	2.51	0.46
3:L:118:GLU:HG2	3:L:119:ILE:H	1.80	0.46
1:A:10:LYS:HB3	1:A:21:TYR:CD2	2.51	0.46
3:L:188:LEU:HD23	3:L:189:SER:N	2.30	0.46
4:H:167:TYR:O	4:H:198:TYR:HB2	2.15	0.46
4:H:20:VAL:HG22	4:H:38:ALA:HB3	1.97	0.46
1:A:55:VAL:HG12	1:A:117:PHE:HE1	1.81	0.46
1:A:11:LYS:HD2	1:A:166:LEU:HD13	1.97	0.46
1:A:325:VAL:O	1:A:344:ALA:HA	2.15	0.46
1:A:10:LYS:HB3	1:A:21:TYR:CE2	2.50	0.46
3:L:220:LYS:HE3	3:L:220:LYS:HB3	1.78	0.46
1:A:7:ARG:HA	1:A:7:ARG:HD2	1.79	0.46
4:H:115:ARG:C	4:H:117:PHE:H	2.19	0.46
1:A:59:CYS:HB2	1:A:144:TYR:CE1	2.51	0.45
1:A:323:VAL:HG12	1:A:347:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:17:MET:O	3:L:112:GLY:HA2	2.16	0.45
1:A:254:ALA:HB2	1:A:276:PRO:HA	1.98	0.45
4:H:113:ARG:HG2	4:H:114:SER:N	2.32	0.45
3:L:52:LYS:HG2	3:L:97:ALA:HB2	1.97	0.45
1:A:208:TYR:O	1:A:351:LEU:HD12	2.17	0.44
3:L:126:PRO:O	3:L:128:VAL:HG23	2.16	0.44
4:H:47:SER:HB3	4:H:113:ARG:HG3	1.99	0.44
3:L:163:VAL:HA	3:L:205:TYR:HA	1.98	0.44
4:H:109:TYR:CD2	4:H:131:VAL:HB	2.52	0.44
4:H:82:ARG:CG	4:H:82:ARG:NH1	2.72	0.44
4:H:125:TRP:CD1	4:H:125:TRP:N	2.85	0.44
1:A:60:ALA:CB	1:A:78:ASP:HA	2.48	0.44
1:A:88:PRO:HB2	1:A:90:ALA:H	1.81	0.44
3:L:91:LEU:HD23	3:L:91:LEU:H	1.82	0.44
3:L:199:TYR:OH	3:L:222:PHE:HE2	2.00	0.44
4:H:86:SER:OG	4:H:95:TYR:HB2	2.18	0.44
1:A:62:ARG:NH1	1:A:138:LYS:HG2	2.32	0.44
1:A:210:HIS:HB2	4:H:117:PHE:CE2	2.53	0.44
1:A:32:ASP:OD1	1:A:32:ASP:N	2.35	0.43
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.81	0.43
1:A:58:THR:OG1	1:A:81:VAL:HG12	2.18	0.43
1:A:178:PRO:HA	1:A:207:ILE:HD12	2.00	0.43
1:A:195:LYS:HB3	1:A:223:ASN:HB3	1.99	0.43
1:A:228:VAL:HB	1:A:262:VAL:HB	2.01	0.43
3:L:63:SER:O	3:L:64:ALA:HB3	2.18	0.43
1:A:214:ILE:O	1:A:273:THR:HA	2.18	0.43
1:A:180:PRO:O	1:A:206:GLU:HB2	2.18	0.43
1:A:147:LYS:HA	1:A:165:ARG:HA	2.01	0.43
1:A:303:SER:OG	1:A:351:LEU:N	2.47	0.43
4:H:62:TRP:HE1	4:H:64:ALA:C	2.22	0.43
4:H:167:TYR:HE1	4:H:171:PRO:HA	1.84	0.43
1:A:220:VAL:HB	1:A:268:PHE:HB3	2.00	0.42
4:H:169:PRO:HG2	4:H:222:HIS:NE2	2.33	0.42
1:A:256:GLU:HG2	1:A:274:LEU:HD11	2.00	0.42
4:H:51:TRP:O	4:H:63:VAL:HG22	2.18	0.42
4:H:91:LYS:HD2	4:H:95:TYR:OH	2.18	0.42
3:L:102:GLN:HG2	3:L:103:GLN:N	2.35	0.42
1:A:210:HIS:CB	4:H:117:PHE:CE2	3.02	0.42
3:L:68:TYR:HB3	3:L:71:VAL:CG2	2.49	0.42
1:A:9:PHE:CD1	1:A:25:ARG:HG2	2.55	0.42
1:A:56:THR:HG22	1:A:147:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:H	1:A:294:LYS:HG2	1.74	0.42
3:L:21:PRO:HG2	3:L:34:ILE:HG23	2.01	0.42
3:L:144:SER:OG	3:L:193:THR:HG23	2.19	0.42
4:H:45:TYR:O	4:H:69:TYR:HB2	2.20	0.42
3:L:20:SER:HB2	3:L:35:THR:CG2	2.48	0.42
1:A:210:HIS:CG	1:A:299:ASN:HD22	2.38	0.42
3:L:129:PHE:CD2	4:H:152:SER:HA	2.55	0.42
1:A:278:LEU:HD12	1:A:278:LEU:O	2.19	0.42
1:A:270:LYS:HD3	1:A:272:TYR:OH	2.20	0.41
3:L:222:PHE:O	3:L:222:PHE:CG	2.70	0.41
4:H:32:SER:OG	4:H:99:ASN:HA	2.20	0.41
1:A:226:LYS:HG2	1:A:330:SER:O	2.20	0.41
1:A:199:LEU:HD23	1:A:345:VAL:HG23	2.03	0.41
1:A:241:ILE:HD12	1:A:241:ILE:N	2.35	0.41
2:V:347:TPO:HA	2:V:348:PRO:HD3	1.95	0.41
3:L:33:THR:CG2	3:L:87:THR:HG22	2.51	0.41
3:L:173:GLN:HB3	4:H:191:VAL:HG11	2.02	0.41
3:L:196:LYS:HB3	3:L:196:LYS:HE2	1.74	0.41
1:A:130:GLN:OE1	1:A:278:LEU:HD11	2.20	0.41
1:A:165:ARG:NH2	2:V:357:SEP:O3P	2.54	0.41
2:V:365:LEU:HG	2:V:366:ARG:H	1.86	0.41
3:L:128:VAL:CG2	3:L:209:VAL:HG21	2.47	0.41
4:H:109:TYR:CE2	4:H:131:VAL:HB	2.55	0.41
3:L:107:VAL:N	3:L:108:PRO:CD	2.84	0.41
4:H:27:VAL:HG11	4:H:101:LEU:HD12	2.03	0.41
1:A:105:ILE:H	1:A:105:ILE:HG13	1.76	0.41
1:A:323:VAL:CG1	1:A:347:LEU:HB2	2.51	0.41
3:L:223:ASN:OD1	3:L:223:ASN:N	2.54	0.41
4:H:54:GLN:HE21	4:H:108:VAL:CG1	2.34	0.41
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.97	0.40
3:L:137:GLN:O	3:L:140:SER:OG	2.34	0.40
4:H:58:LYS:HB2	4:H:58:LYS:HE2	1.91	0.40
1:A:138:LYS:HD2	1:A:138:LYS:HA	1.87	0.40
4:H:113:ARG:HG2	4:H:114:SER:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/426 (82%)	320 (92%)	28 (8%)	0	100	100
2	V	11/23 (48%)	7 (64%)	4 (36%)	0	100	100
3	L	210/227 (92%)	181 (86%)	29 (14%)	0	100	100
4	H	209/249 (84%)	185 (88%)	24 (12%)	0	100	100
All	All	778/925 (84%)	693 (89%)	85 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/380 (77%)	277 (95%)	15 (5%)	24	54
2	V	9/15 (60%)	9 (100%)	0	100	100
3	L	172/199 (86%)	161 (94%)	11 (6%)	17	47
4	H	148/209 (71%)	141 (95%)	7 (5%)	26	57
All	All	621/803 (77%)	588 (95%)	33 (5%)	22	53

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	117	PHE
1	A	124	PRO
1	A	153	ASN
1	A	192	MET
1	A	218	VAL
1	A	226	LYS
1	A	237	GLN
1	A	249	TYR
1	A	253	VAL
1	A	261	THR
1	A	285	ARG
1	A	303	SER
1	A	335	LEU
3	L	25	SER
3	L	36	CYS
3	L	40	GLN
3	L	69	SER
3	L	73	SER
3	L	90	SER
3	L	91	LEU
3	L	95	ASP
3	L	192	LEU
3	L	194	LEU
3	L	223	ASN
4	H	67	SER
4	H	73	THR
4	H	82	ARG
4	H	89	THR
4	H	93	THR
4	H	133	VAL
4	H	218	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	299	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPO	V	360	2	8,10,11	1.21	1 (12%)	10,14,16	1.88	2 (20%)
2	SEP	V	357	2	8,9,10	1.73	1 (12%)	8,12,14	1.58	2 (25%)
2	TPO	V	359	2	8,10,11	1.76	2 (25%)	10,14,16	1.53	1 (10%)
2	SEP	V	362	2	8,9,10	1.63	1 (12%)	8,12,14	1.83	3 (37%)
2	SEP	V	350	2	8,9,10	1.64	2 (25%)	8,12,14	2.10	2 (25%)
2	TPO	V	347	2	8,10,11	1.74	2 (25%)	10,14,16	1.79	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	V	360	2	-	1/9/11/13	-
2	SEP	V	357	2	-	4/5/8/10	-
2	TPO	V	359	2	-	4/9/11/13	-
2	SEP	V	362	2	-	3/5/8/10	-
2	SEP	V	350	2	-	2/5/8/10	-
2	TPO	V	347	2	-	1/9/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	357	SEP	P-O1P	3.84	1.62	1.50
2	V	359	TPO	P-O1P	3.52	1.61	1.50
2	V	347	TPO	P-O1P	3.48	1.61	1.50
2	V	350	SEP	P-O1P	3.40	1.61	1.50
2	V	362	SEP	P-O1P	3.29	1.61	1.50
2	V	347	TPO	P-OG1	2.26	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	350	SEP	P-O3P	2.10	1.62	1.54
2	V	360	TPO	P-O2P	2.09	1.62	1.54
2	V	359	TPO	P-O3P	2.08	1.62	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	360	TPO	P-OG1-CB	-4.83	108.61	123.21
2	V	359	TPO	P-OG1-CB	-4.22	110.46	123.21
2	V	350	SEP	OG-CB-CA	4.22	112.25	108.14
2	V	362	SEP	OG-CB-CA	3.87	111.91	108.14
2	V	347	TPO	P-OG1-CB	-3.65	112.19	123.21
2	V	347	TPO	CG2-CB-CA	-3.37	106.51	113.16
2	V	357	SEP	P-OG-CB	-3.32	109.16	118.30
2	V	350	SEP	P-OG-CB	-3.09	109.78	118.30
2	V	362	SEP	O3P-P-OG	2.58	113.59	106.73
2	V	357	SEP	OG-CB-CA	2.56	110.64	108.14
2	V	360	TPO	CG2-CB-CA	-2.42	108.40	113.16
2	V	347	TPO	O-C-CA	-2.15	119.16	124.78
2	V	362	SEP	P-OG-CB	-2.12	112.46	118.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	350	SEP	N-CA-CB-OG
2	V	350	SEP	CA-CB-OG-P
2	V	357	SEP	CB-OG-P-O1P
2	V	357	SEP	CB-OG-P-O2P
2	V	357	SEP	CB-OG-P-O3P
2	V	359	TPO	N-CA-CB-OG1
2	V	359	TPO	C-CA-CB-CG2
2	V	359	TPO	O-C-CA-CB
2	V	362	SEP	CB-OG-P-O2P
2	V	362	SEP	CB-OG-P-O3P
2	V	362	SEP	CB-OG-P-O1P
2	V	359	TPO	N-CA-CB-CG2
2	V	357	SEP	CA-CB-OG-P
2	V	347	TPO	CB-OG1-P-O3P
2	V	360	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	357	SEP	1	0
2	V	347	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	356/426 (83%)	0.17	4 (1%) 80 80	69, 107, 140, 169	0
2	V	14/23 (60%)	0.44	0 100 100	108, 133, 150, 157	0
3	L	212/227 (93%)	0.30	10 (4%) 31 29	91, 126, 149, 164	0
4	H	213/249 (85%)	0.11	7 (3%) 46 44	75, 107, 148, 166	0
All	All	795/925 (85%)	0.19	21 (2%) 56 52	69, 113, 147, 169	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	221	ASN	4.3
4	H	202	SER	4.1
4	H	176	TRP	3.6
3	L	146	VAL	3.0
3	L	72	PRO	2.9
4	H	180	ALA	2.7
1	A	199	LEU	2.6
3	L	95	ASP	2.5
3	L	117	VAL	2.5
3	L	169	SER	2.4
3	L	149	LEU	2.4
3	L	147	CYS	2.3
3	L	218	VAL	2.3
4	H	174	VAL	2.2
1	A	200	GLU	2.2
4	H	101	LEU	2.2
4	H	206	VAL	2.1
3	L	165	ASN	2.1
1	A	122	ASN	2.1
3	L	91	LEU	2.1
1	A	41	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TPO	V	347	11/12	0.71	0.26	136,142,154,157	0
2	TPO	V	359	11/12	0.83	0.26	128,144,165,172	0
2	SEP	V	350	10/11	0.90	0.24	117,125,131,132	0
2	SEP	V	362	10/11	0.91	0.20	95,102,119,120	0
2	TPO	V	360	11/12	0.93	0.20	107,115,122,123	0
2	SEP	V	357	10/11	0.93	0.30	134,138,151,152	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.